STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 152212

TO: Rei-Tsang Shiao
Location: 5a10 / 5c18
Tuesday, May 03, 2005
Art Unit: 1626
Phone: 571-272-0707
Serial Number: 10 / 678626

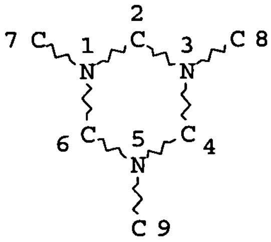
From: Jan Delaval
Location: Biotech-Chem Library
Remsen 1a51
Phone: 571-272-~~2~~2504

jan.delaval@uspto.gov

Search Notes

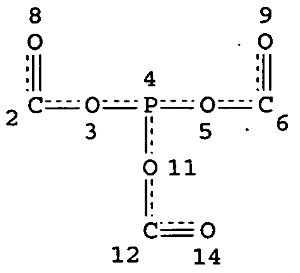
sira
Search and Information Resources Administration

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 09:00:59 ON 03 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     2 MAY 2005  HIGHEST RN 849658-68-0
DICTIONARY FILE UPDATES:    2 MAY 2005  HIGHEST RN 849658-68-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*******************************************************************
*                                                                 *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                 *
*******************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l28
L26             STR
```

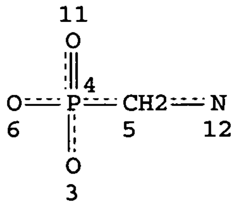


```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
L28       11337 SEA FILE=REGISTRY SSS FUL L26

100.0% PROCESSED  50585 ITERATIONS                  11337 ANSWERS
SEARCH TIME: 00.00.01
```

```
=> d sta que l34
L32                STR
```



```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L34           44 SEA FILE=REGISTRY SSS FUL L32

100.0% PROCESSED   6955 ITERATIONS                          44 ANSWERS
SEARCH TIME: 00.00.01



=> d sta que l38
L36                STR
```



```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   6

STEREO ATTRIBUTES: NONE
L38         8960 SEA FILE=REGISTRY SSS FUL L36

100.0% PROCESSED  39084 ITERATIONS                        8960 ANSWERS
SEARCH TIME: 00.00.01



=> d his

     (FILE 'HOME' ENTERED AT 08:39:10 ON 03 MAY 2005)
                SET COST OFF
     FILE 'HCAPLUS' ENTERED AT 08:40:08 ON 03 MAY 2005
L1            1 S US20040092765/PN OR (US2003-678626# OR WO2000-EP13162 OR US20
                E WULFF C/AU
L2           56 S E3,E4,E9,E10
                E ORSTEN S/AU
L3            8 S E4
                E OFTRING A/AU
L4          130 S E3,E4
                E OEFTRING A/AU
                E OFFTRING/AU
L5            4 S L2-L4 AND ?PHOSPHONOMETHYLGLYCIN?
L6           16 S L2-L4 AND ?GLYCIN?
L7            5 S L6 AND ?PHOSPH?
L8            5 S L5,L7
L9            4 S L2-L4 AND ?PHOSPHONOMETHYL GLYCIN?
L10           0 S L2-L4 AND ?PHOSPHONO METHYL GLYCIN?
L11           0 S L2-L4 AND ?PHOSPHONO METHYLGLYCIN?
L12           5 S L8,L9
                SEL RN

     FILE 'REGISTRY' ENTERED AT 08:47:11 ON 03 MAY 2005
L13         118 S E1-E118
L14           1 S 1071-83-6
L15         739 S 1071-83-6/CRN

     FILE 'HCAPLUS' ENTERED AT 08:47:33 ON 03 MAY 2005
L16        5180 S L14
L17        1411 S L15
L18           5 S L2-L4 AND L16,L17
L19           5 S L12,L18

     FILE 'REGISTRY' ENTERED AT 08:47:53 ON 03 MAY 2005
L20           1 S L13 AND L14,L15
L21         117 S L13 NOT L20
L22           8 S L21 AND NCNCNC/ES
L23          15 S L21 AND P/ELS
L24           3 S L23 AND O>=6
L25           2 S L24 NOT N/ELS
L26             STR
L27          50 S L26
L28       11337 S L26 FUL
L29           1 S L22 AND C9H12N6
L30       11337 S L28,L29
L31           2 S L22 NOT L30
L32             STR
L33           3 S L32
L34          44 S L32 FUL
                SAV L28 SHIAO678A/A
                SAV L34 SHIAO678B/A
L35             STR
L36             STR L35
L37          50 S L36
L38        8960 S L36 FUL
                SAV L38 SHIAO678C/A
L39           0 S L35 FUL SUB=L38
L40           9 S L13 AND L38
L41           2 S L13 AND L34

     FILE 'HCAPLUS' ENTERED AT 08:57:41 ON 03 MAY 2005
L42       14182 S L30
L43          50 S L34
L44           2 S L42 AND L43
L45           2 S L44 AND L16,L17
```

```
L46            2 S L44 AND L38
L47            2 S L44 AND (?PHOSPHONOMETHYLGLYCIN? OR ?PHOSPHONOMETHYL GLYCIN?
L48            2 S L44-L47
L49            2 S L48 AND L1-L12
L50            2 S L19 AND L49
L51            3 S L19 NOT L50
L52            4 S L1-L12 AND L42
L53            2 S L1-L12 AND L43
L54            5 S L1-L12 AND L38
L55            5 S L12,L19,L50-L54

     FILE 'REGISTRY' ENTERED AT 09:00:59 ON 03 MAY 2005

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 09:01:32 ON 03 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
the American Chemical Society and is provided to assist you in searching
databases on STN. Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 3 May 2005  VOL 142 ISS 19
FILE LAST UPDATED: 2 May 2005  (20050502/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d l55 all hitstr tot

L55  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:631237  HCAPLUS
DN   141:174162
ED   Entered STN:  06 Aug 2004
TI   Preparation of cosurfactants with unsaturated heterocyclic head groups
IN   Noerenberg, Ralf; Wulff, Christian; Tropsch, Juergen;
     Scholtissek, Martin
PA   BASF AG, Germany
SO   Ger. Offen., 32 pp.
     CODEN: GWXXBX
DT   Patent
LA   German
IC   ICM  C07D263-10
     ICS  C07D233-04; C07D277-08; C07D265-08; C07D239-06; C07D279-06;
          C11D001-58; A61K007-06; A61K007-50
CC   28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 46, 62, 63
FAN.CNT 1
     PATENT NO.          KIND    DATE        APPLICATION NO.        DATE
     ---------------     ----    --------    --------------------   --------
PI   DE 10302905          A1     20040805    DE 2003-10302905       20030124
     WO 2004065373        A1     20040805    WO 2004-EP513          20040122
         W:  AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG,
```

BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR,
CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES,
ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN,
IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC,
LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX,
MZ, MZ, NA, NI

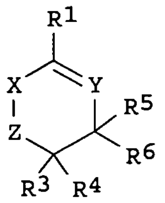
PRAI DE 2003-10302905 A 20030124

CLASS

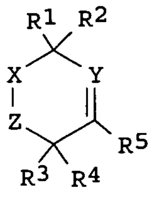
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
DE 10302905	ICM	C07D263-10
	ICS	C07D233-04; C07D277-08; C07D265-08; C07D239-06; C07D279-06; C11D001-58; A61K007-06; A61K007-50
DE 10302905	ECLA	C07D233/14; C07D263/14
WO 2004065373	ECLA	C07D233/14; C07D263/14

OS CASREACT 141:174162; MARPAT 141:174162

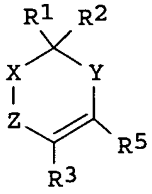
GI



I



II



III

AB The present invention concerns compds., e.g., I [X = O, S, NR24; Y = N (for I and II), NR24 (for III); Z = CR7R8; R1 = (un)branched, (un)substituted C3-29-alkyl, C3-29-alkenyl; R2 = H, Me; R3, R4, R5, R6 = H, CN, CO2H, CO2R18, CONR19R20, (un)substituted Ph; R7, R8 = H, CN, CO2H, CO2R18, NR19R20, (un)substituted Ph; R16, R17 = H, (un)branched C1-4-alkyl; R18 = C1-6-alkyl, (CH2CH2O)p; R19, R20 = H, (un)branched C1-4-alkyl; R22 = C1-10-alkyl, COR23, (CH2CH2O)q, (CHMeCH2O)r, (CH2CH2CH2CH2O)s; R23 = C1-18-alkyl; R24 = H, C1-4-alkyl {optionally substituted at C(3) with OH, NH2, OR22, NR16R17}; n = 0, 1; p = 1 - 15; q = 1 - 15; r = 1 -15; s = 1 - 15], II and III, with unsatd. hetero-cyclic head groups procedures for the production of the compds. according to invention by conversion of aldehydes or carbonic acids and/or their derivs. with polyfunctional compds., which contain at least one amino function and at least a further function from the group the hydroxyl -, diol -, amino carboxyl functions, their use as cosurfactants as well as household detergent, household cleaner, body cleaning agent or toiletry, containing at least a compound according to invention. Thus, 2-(1-Ethylpentyl)1-4-methyl-4-(hydroxymethyl)-4,5-dihydrooxazole [I; X = O, Y = N, Z = bond, R1 = CHEtBu, R3 = R4 = H, R5 = Me, R6 = CH2OH] was prepared via cyclocondensation of BuCHEtCO2H with MeC(NH2)(CH2OH)2. The cosurfactant I [X = O, Y = N, Z = bond, R1 = CHEtBu, R3 = R4 = H, R5 = Me, R6 = CH2(OCH2CH2)nOH, n = 3, 6, 10] is then prepared via reaction of I [X = O, Y = N, Z = bond, R1 = CHEtBu, R3 = R4 = H, R5 = Me, R6 = CH2OH] with ethylene oxide in aqueous KOH solution

ST heterocyclic compd unsatd cosurfactant prepn detergent toiletry

IT Carbohydrates, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amino sugars, cyclocondensation of, with aldehydes and carboxylic acids; preparation of cosurfactants with unsatd. heterocyclic head groups)

IT Alcohols, reactions
Thiols (organic), reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

```
        (amino, cyclocondensation of, with aldehydes and carboxylic acids;
        preparation of cosurfactants with unsatd. heterocyclic head groups)
IT   Hygiene
        (body cleaning agent for; preparation of cosurfactants with unsatd.
        heterocyclic head groups for)
IT   Detergents
        (cleaning compns.; preparation of cosurfactants with unsatd. heterocyclic
        head groups for)
IT   Surfactants
        (co-surfactants; preparation of cosurfactants with unsatd. heterocyclic head
        groups)
IT   Hair preparations
        (conditioners, styling; preparation of cosurfactants with unsatd.
        heterocyclic head groups for)
IT   Cosmetics
        (creams; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Ion exchangers
        (cyclocondensation catalyst; preparation of cosurfactants with unsatd.
        heterocyclic head groups)
IT   Bronsted acids
     Lewis acids
     RL: CAT (Catalyst use); USES (Uses)
        (cyclocondensation catalyst; preparation of cosurfactants with unsatd.
        heterocyclic head groups)
IT   Amino acids, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with aldehydes and carboxylic acids; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
IT   Aldehydes, reactions
     Carboxylic acids, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with amino alcs.; preparation of cosurfactants with
        unsatd. heterocyclic head groups)
IT   Gels
     Granular materials
     Liquids
     Powders
     Solids
     Tablets
        (detergent formulations; preparation of cosurfactants with unsatd.
        heterocyclic head groups for)
IT   Detergents
        (dishwashing; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Bath preparations
        (douches; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Hair preparations
        (dyes; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Detergents
        (floor cleaners; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Degreasing agents
        (for metal; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Bath preparations
     Cosmetics
     Hair preparations
        (gels; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Detergents
```

```
        (granular; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Cosmetics
        (hand creams, cleansing; preparation of cosurfactants with unsatd.
        heterocyclic head groups for)
IT   Detergents
        (household; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Heterocyclic compounds
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (isoxazoles, preparation and reaction of, with ethylene oxide; preparation
of
        cosurfactants with unsatd. heterocyclic head groups)
IT   Cosmetics
        (lipsticks; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Cosmetics
        (liqs.; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Bath preparations
        (lotions and tablets; preparation of cosurfactants with unsatd. heterocyclic
        head groups for)
IT   Hair preparations
        (lotions; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Cyclocondensation reaction
        (of carboxylic acids and aldehydes with amino alcs.; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
IT   Polymerization
        (oligomerization, of ethylene oxide in the presence of
        hydroxymethylated heterocyclic compds.; preparation of cosurfactants with
        unsatd. heterocyclic head groups)
IT   Cosmetics
        (powders; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Shampoos
        (preparation of cosurfactants with unsatd. heterocyclic head groups for)
IT   Cosmetics
        (skin care and toiletry; preparation of cosurfactants with unsatd.
        heterocyclic head groups for)
IT   Detergents
        (skin cleansers; preparation of cosurfactants with unsatd. heterocyclic head
        groups for)
IT   Cosmetics
        (solids; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Hair preparations
        (sprays; preparation of cosurfactants with unsatd. heterocyclic head groups
        for)
IT   Amines, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (thiol, cyclocondensation of, with aldehydes and carboxylic acids;
        preparation of cosurfactants with unsatd. heterocyclic head groups)
IT   104-15-4, p-Toluenesulfonic acid, uses   7664-93-9, Sulfuric acid, uses
     24057-28-1, Pyridinium p-tosylate
     RL: CAT (Catalyst use); USES (Uses)
        (cyclocondensation catalyst; preparation of cosurfactants with unsatd.
        heterocyclic head groups)
IT   149-57-5, 2-Ethylhexanoic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with 2-amino-2-alkyl-1,3-propanediol; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
```

```
IT   77-86-1, [Tris(hydroxymethyl)methyl]amine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with 2-ethylhexanal; preparation of cosurfactants
        with unsatd. heterocyclic head groups)
IT   115-69-5, 2-Amino-2-methyl-1,3-propanediol   115-70-8,
     2-Amino-2-ethyl-1,3-propanediol
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with 2-ethylhexanoic acid; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
IT   123-05-7, 2-Ethylhexanal
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with [tris(hydroxymethyl)methyl]amine; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
IT   52-90-4, L-Cysteine, reactions   56-40-6, Glycine, reactions
     56-41-7, L-Alanine, reactions   56-45-1, L-Serine, reactions   56-84-8,
     L-Asparaginic acid, reactions   56-85-9, L-Glutamine, reactions   56-86-0,
     L-Glutaminic acid, reactions   56-87-1, L-Lysine, reactions   56-89-3,
     L-Cystine, reactions   60-18-4, L-Tyrosine, reactions   61-90-5,
     L-Leucine, reactions   63-68-3, L-Methionine, reactions   63-91-2,
     L-Phenylalanine, reactions   70-47-3, L-Asparagine, reactions   71-00-1,
     L-Histidine, reactions   72-18-4, L-Valine, reactions   72-19-5,
     L-Threonine, reactions   73-22-3, L-Tryptophan, reactions   73-32-5,
     L-Isoleucine, reactions   74-79-3, L-Arginine, reactions   78-90-0,
     Propylenediamine   111-40-0, Diethylenetriamine   111-41-1,
     N-(2-Hydroxyethyl)ethylenediamine   111-42-2, Diethanolamine, reactions
     112-24-3, Triethylenetetramine   142-73-4, Iminodiacetic acid   147-85-3,
     L-Proline, reactions   156-87-6, Propanolamine   462-47-5,
     3-Mercaptopropylamine   688-57-3, Ethylenediaminetriacetic acid
     1071-83-6, N-(Phosphonomethyl)glycine
     10563-26-5, N,N'-Bis(3-aminopropyl)ethylenediamine   13531-52-7,
     N-(3-Aminopropyl)ethylenediamine   85305-25-5, Dipropanolamine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with aldehydes and carboxylic acids; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
IT   75-21-8, Ethylene oxide, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oligomerization of, with hydroxymethylated heterocyclic compds.;
        preparation of cosurfactants with unsatd. heterocyclic head groups)
IT   24498-17-7P, 2-(1-Ethylpentyl)-4-ethyl-4-(hydroxymethyl)-4,5-
     dihydrooxazole   651291-16-6P, 2-(1-Ethylpentyl)-4,4-di(hydroxymethyl)-4,5-
     dihydrooxazole   731859-24-8P, 2-(1-Ethylpentyl)-4-methyl-4-
     (hydroxymethyl)-4,5-dihydrooxazole
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, with ethylene oxide; preparation of
cosurfactants
        with unsatd. heterocyclic head groups)
IT   270263-28-0P   731859-32-8P   731859-35-1P   731859-38-4P   731859-41-9P
     731859-43-1P   731859-45-3P   731859-47-5P   731859-49-7P   731859-51-1P
     731859-54-4P   731859-56-6P   731859-58-8P   731859-60-2P   731859-62-4P
     731859-64-6P   731859-66-8P   731859-68-0P   731859-70-4P   731859-72-6P
     731859-74-8P   731859-76-0P   731859-78-2P   731859-80-6P   731859-82-8P
     731859-84-0P   731859-86-2P   731859-87-3P   731859-88-4P   731859-89-5P
     731859-90-8P   731859-92-0P   731859-94-2P   731859-95-3P   731859-96-4P
     731859-97-5P   731859-98-6P   731859-99-7P
     RL: COS (Cosmetic use); MOA (Modifier or additive use); NUU (Other use,
     unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP
     (Preparation); USES (Uses)
        (preparation of cosurfactants with unsatd. heterocyclic head groups)
IT   1071-83-6, N-(Phosphonomethyl)glycine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation of, with aldehydes and carboxylic acids; preparation of
        cosurfactants with unsatd. heterocyclic head groups)
```

```
RN   1071-83-6  HCAPLUS
CN   Glycine, N-(phosphonomethyl)- (7CI, 8CI, 9CI)  (CA INDEX NAME)
```

$HO_2C-CH_2-NH-CH_2-PO_3H_2$

```
L55  ANSWER 2 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2003:5971  HCAPLUS
DN   138:56081
ED   Entered STN:  05 Jan 2003
TI   Method for producing N-phosphonomethylglycine by the reaction of
     hexahydrotriazine with triacyl phosphate in organic solvent and
     removing the soluble impurities
IN   Vandenmersch, Hugues; Voss, Hartwig; Orsten, Stefan; Wulff,
     Christian
PA   BASF Aktiengesellschaft, Germany
SO   PCT Int. Appl., 17 pp.
     CODEN: PIXXD2
DT   Patent
LA   German
IC   ICM  C07F009-38
CC   29-7 (Organometallic and Organometalloidal Compounds)
FAN.CNT 1
     PATENT NO.          KIND   DATE       APPLICATION NO.        DATE
     ---------------     ----   --------   --------------------   --------
PI   WO 2003000704        A2    20030103   WO 2002-EP6903         20020621
     WO 2003000704        A3    20030501
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10130136          A1    20030102   DE 2001-10130136       20010622
     EP 1401846           A2    20040331   EP 2002-754734         20020621
     EP 1401846           B1    20041215
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002010569        A     20040803   BR 2002-10569          20020621
     NZ 530049            A     20040827   NZ 2002-530049         20020621
     JP 2004535438        T2    20041125   JP 2003-507107         20020621
     AT 284890            E     20050115   AT 2002-754734         20020621
     TW 575579            B     20040211   TW 2002-91113652       20021018
     US 2004235664        A1    20041125   US 2003-481565         20031222
PRAI DE 2001-10130136     A     20010622
     WO 2002-EP6903       W     20020621
CLASS
 PATENT NO.      CLASS  PATENT FAMILY CLASSIFICATION CODES
 -------------   -----  ----------------------------------------------
 WO 2003000704   ICM    C07F009-38
 DE 10130136     ECLA   C07F009/38A1+U6F
 JP 2004535438   FTERM  4D006/GA03; 4D006/KA16; 4D006/KA53; 4D006/KA54;
                        4D006/KA55; 4D006/KA56; 4D006/KA63; 4D006/KA67;
                        4D006/KE04Q; 4D006/KE06Q; 4D006/KE15P; 4D006/KE15Q;
                        4D006/MA06; 4D006/MA11; 4D006/MB05; 4D006/MC02;
                        4D006/MC03; 4D006/MC05; 4D006/MC54; 4D006/PA01;
                        4D006/PB70; 4D006/PC80; 4H050/AA02; 4H050/AD15;
```

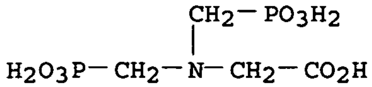
N

(10481565)

```
                     4H050/AD19; 4H050/BB31; 4H050/BE01; 4H050/BE10
 US 2004235664  NCL  504/206.000; 562/017.000
                ECLA C07F009/38A1+U6F
OS   CASREACT 138:56081; MARPAT 138:56081
AB   The invention relates to a method for producing N-
     phosphonomethylglycine from an aqueous mixture containing N-
     phosphonomethylglycine, ammonium halogenides and alkali halides or
     earth alkali halides and optionally, organic impurities in a dissolved form.
     According to the invention, (a) the pH-value of the mixture is regulated to
     a value of 2-8, (b) the mixture is separated by means of a selective
     nanofiltration membrane, to obtain a retentate rich in N-
     phosphonomethylglycine and poor in halogenides and a permeate rich
     in halogenides and poor in N-phosphonomethylglycine and (c) the
     N-phosphonomethylglycine is prepared from the retentate.  The
     inventive method enables the production of N-phosphonomethylglycine
     by simultaneously separating the halogenide salts thereof.  Thus, reaction of
     ammonium benzoate with PCl3 in 1,2-dichloroethane below 36° for 30
     min followed by treatment with 1,3,5-Tris(cyanomethyl)-1,3,5-
     triazacyclohexane and hydrolysis with aqueous HCl gave title compound
along-with
     aminomethylphosphonic acid, bis(phosphinomethyl)
     glycine, glycine, NaCl/NH4Cl as dissolved impurities.
ST   N phosphonomethyl glycine prepn purifn; triacyl
     phosphate reaction hexahydrotriazine;
     phosphonomethylglycine prepn purifn
IT   Impurities
        (method for producing N-phosphonomethylglycine by the
        reaction of hexahydrotriazine with triacyl phosphate in organic
        solvent and removing the soluble impurities)
IT   56-40-6P, Glycine, preparation 1066-51-9P,
     Aminomethylphosphonic acid 2439-99-8P, N,N-Bis(
     phosphonomethyl)glycine
     RL: BYP (Byproduct); PREP (Preparation)
        (method for producing N-phosphonomethylglycine by the
        reaction of hexahydrotriazine with triacyl phosphate in organic
        solvent and removing the soluble impurities)
IT   1863-63-4, Ammonium benzoate 4560-87-6, 1,3,5-Tris(cyanomethyl)-
     1,3,5-triazacyclohexane   7719-12-2, Phosphorus chloride (PCl3)
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (method for producing N-phosphonomethylglycine by the
        reaction of hexahydrotriazine with triacyl phosphate in organic
        solvent and removing the soluble impurities)
IT   1071-83-6P, N-Phosphonomethylglycine
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (method for producing N-phosphonomethylglycine by the
        reaction of hexahydrotriazine with triacyl phosphate in organic
        solvent and removing the soluble impurities)
IT   107-06-2, 1,2-Dichloroethane, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (solvent; method for producing N-phosphonomethylglycine by
        the reaction of hexahydrotriazine with triacyl phosphate in
        organic solvent and removing the soluble impurities)
IT   1066-51-9P, Aminomethylphosphonic acid
     2439-99-8P, N,N-Bis(phosphonomethyl)glycine
     RL: BYP (Byproduct); PREP (Preparation)
        (method for producing N-phosphonomethylglycine by the
        reaction of hexahydrotriazine with triacyl phosphate in organic
        solvent and removing the soluble impurities)
RN   1066-51-9  HCAPLUS
CN   Phosphonic acid, (aminomethyl)- (6CI, 7CI, 8CI, 9CI)   (CA INDEX NAME)
```

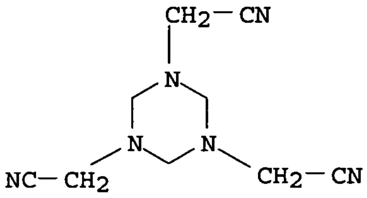
$H_2N-CH_2-PO_3H_2$

RN 2439-99-8 HCAPLUS
CN Glycine, N,N-bis(phosphonomethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



$$\begin{array}{l} \qquad\quad\; CH_2-PO_3H_2 \\ \qquad\quad\;\, | \\ H_2O_3P-CH_2-N-CH_2-CO_2H \end{array}$$

IT **4560-87-6**, 1,3,5-Tris(cyanomethyl)-1,3,5-triazacyclohexane
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for producing N-**phosphonomethylglycine** by the reaction of hexahydrotriazine with triacyl **phosphate** in organic solvent and removing the soluble impurities)
RN 4560-87-6 HCAPLUS
CN 1,3,5-Triazine-1,3,5(2H,4H,6H)-triacetonitrile (9CI) (CA INDEX NAME)



IT **1071-83-6P**, N-**Phosphonomethylglycine**
RL: SPN (Synthetic preparation); PREP (Preparation)
(method for producing N-**phosphonomethylglycine** by the reaction of hexahydrotriazine with triacyl **phosphate** in organic solvent and removing the soluble impurities)
RN 1071-83-6 HCAPLUS
CN Glycine, N-(phosphonomethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

$HO_2C-CH_2-NH-CH_2-PO_3H_2$

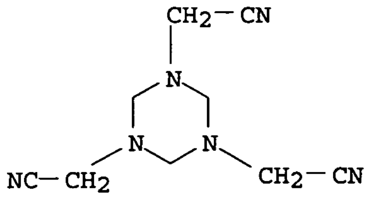
L55 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:5970 HCAPLUS
DN 138:56080
ED Entered STN: 05 Jan 2003
TI Method for producing N-**phosphonomethylglycine** by the reaction of hexahydrotriazine with triacyl **phosphate** in organic solvent
IN **Wulff, Christian**; **Orsten, Stefan**; **Oftring, Alfred**; Zehner, Peter
PA BASF Aktiengesellschaft, Germany
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM C07F009-38
ICS C07F009-40
CC 29-7 (Organometallic and Organometalloidal Compounds)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

```
PI   WO 2003000703         A1    20030103    WO 2002-EP6902         20020621
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
            TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
            CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10130135           A1    20030102    DE 2001-10130135       20010622
     EP 1401845            A1    20040331    EP 2002-754733         20020621
     EP 1401845            B1    20050413
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002010529         A     20040622    BR 2002-10529          20020621
     NZ 530026             A     20040730    NZ 2002-530026         20020621
     JP 2004532282         T2    20041021    JP 2003-507106         20020621
     US 2004236145         A1    20041125    US 2003-481579         20031222
PRAI DE 2001-10130135      A     20010622
     WO 2002-EP6902        W     20020621
CLASS
 PATENT NO.      CLASS  PATENT FAMILY CLASSIFICATION CODES
 -------------   -----  ----------------------------------------------
 WO 2003000703   ICM    C07F009-38
                 ICS    C07F009-40
 WO 2003000703   ECLA   C07F009/38A1+U6F; C07F009/40C9Q
 DE 10130135     ECLA   C07F009/38A1+U6F; C07F009/40C9Q
 JP 2004532282   FTERM  4H050/AA02; 4H050/AC40; 4H050/AD15; 4H050/AD16;
                        4H050/BB12; 4H050/BB14; 4H050/BB31; 4H050/BC10;
                        4H050/BC16; 4H050/BD35; 4H050/BD52; 4H050/BE01;
                        4H050/BE10; 4H050/WA11; 4H050/WA13; 4H050/WA24;
                        4H050/WA26
 US 2004236145   NCL    562/018.000
                 ECLA   C07F009/38A1+U6F; C07F009/40C9Q
OS   CASREACT 138:56080; MARPAT 138:56080
AB   The invention relates to a method for producing N-
     phosphonomethylglycine by reacting a hexahydrotriazine compound with
     a triacyl phosphate in an organic solvent and the saponification of the
     phosphono compound which is obtained after previous extraction into an
     aqueous phase, and separation of the organic phase.  According to the
invention, said
     method prevents decomposition of the organic solvent during saponification
Thus, reaction
     of ammonium benzoate with PCl3 in 1,2-dichloroethane below 36° for
     30 min followed by treatment with 1,3,5-Tris(cyanomethyl)-1,3,5-
     triazacyclohexane and hydrolysis with H2O gave title compound
ST   N phosphonomethyl glycine prepn; triacyl
     phosphate reaction hexahydrotriazine;
     phosphonomethylglycine prepn
IT   1863-63-4, Ammonium benzoate 4560-87-6, 1,3,5-Tris(cyanomethyl)-
     1,3,5-triazacyclohexane   7719-12-2, Phosphorus chloride (PCl3)
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (method for producing N-phosphonomethylglycine by reaction of
        hexahydrotriazine with triacyl phosphate in organic solvent)
IT   1071-83-6P, N-Phosphonomethylglycine
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (method for producing N-phosphonomethylglycine by reaction of
        hexahydrotriazine with triacyl phosphate in organic solvent)
IT   107-06-2, 1,2-Dichloroethane, uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (solvent; method for producing N-phosphonomethylglycine by
```

ND

reaction of hexahydrotriazine with triacyl **phosphate** in organic
solvent)
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Basf Ag; WO 0147938 A 2001 HCAPLUS
(2) Ha, H; US 5053529 A 1991 HCAPLUS
(3) Stauffer Chemical Co; EP 0097522 A 1984 HCAPLUS
(4) Stauffer Chemical Co; EP 0104775 A 1984 HCAPLUS
(5) Stauffer Chemical Co; EP 0149294 A 1985 HCAPLUS
IT **4560-87-6**, 1,3,5-Tris(cyanomethyl)-1,3,5-triazacyclohexane
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for producing N-**phosphonomethylglycine** by reaction of
hexahydrotriazine with triacyl **phosphate** in organic solvent)
RN 4560-87-6 HCAPLUS
CN 1,3,5-Triazine-1,3,5(2H,4H,6H)-triacetonitrile (9CI) (CA INDEX NAME)

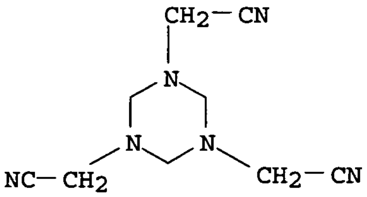


IT **1071-83-6P**, N-**Phosphonomethylglycine**
RL: SPN (Synthetic preparation); PREP (Preparation)
(method for producing N-**phosphonomethylglycine** by reaction of
hexahydrotriazine with triacyl **phosphate** in organic solvent)
RN 1071-83-6 HCAPLUS
CN Glycine, N-(phosphonomethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

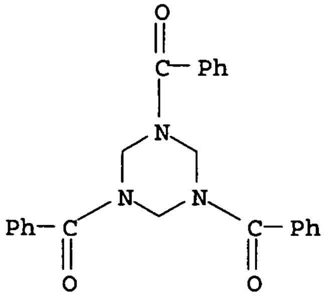
$HO_2C-CH_2-NH-CH_2-PO_3H_2$

L55 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:5969 HCAPLUS
DN 138:56079
ED Entered STN: 05 Jan 2003
TI Method for producing α- **aminophosphonic** acids by the
reaction of hexahydro triazine derivative with triorgano **phosphate**
IN **Wulff, Christian**; **Orsten, Stefan**; **Oftring,
Alfred**
PA BASF Aktiengesellschaft, Germany
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM C07F009-38
ICS C07F009-40
CC 29-7 (Organometallic and Organometalloidal Compounds)
FAN.CNT 1

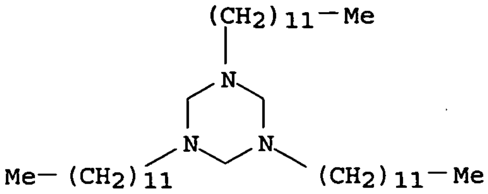
```
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
PI   WO 2003000702        A1    20030103    WO 2002-EP6901         20020621
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10130134          A1     20030102    DE 2001-10130134        20010622
     EP 1401847           A1     20040331    EP 2002-780837          20020621
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002010528        A      20040622    BR 2002-10528           20020621
     US 2004236144        A1     20041125    US 2003-481576          20031222
PRAI DE 2001-10130134     A      20010622
     WO 2002-EP6901       W      20020621
CLASS
 PATENT NO.      CLASS  PATENT FAMILY CLASSIFICATION CODES
 -------------   -----  ----------------------------------------
 WO 2003000702   ICM    C07F009-38
                 ICS    C07F009-40
 DE 10130134     ECLA   C07F009/38A1+U; C07F009/38A1+U6F; C07F009/40C9Q
 US 2004236144   NCL    562/016.000
                 ECLA   C07F009/38A1+U; C07F009/38A1+U6F; C07F009/40C9Q
OS   CASREACT 138:56079; MARPAT 138:56079
AB   The invention relates to a method for producing α-
     aminophosphonic acids, by reacting a hexahydro triazine derivative
     with a triorgano phosphate. The inventive method includes a
     phosphono compound as an intermediate step, said phosphono
     compound being hydrolyzed into α- aminophosphonic acid. The
     invention also relates to said phosphono compound and the method
     for the production thereof. Thus, reaction of PCl3 with sodium benzoate in
     1,4-dioxane followed by treatment with 1,3,5-tris(cyanomethyl)-1,3,5-
     triazacyclohexane and aqueous HCl hydrolysis gave 91%
     phosphonomethylglycine in 95.3% purity. The inventive method
     enables α- aminophosphonic acids to be produced in a simple
     and economical manner as well as ensuring a high yield and purity.
ST   aminophosphonic acid prepn; hexahydro triazine deriv reaction
     triorgano phosphate; aminomethylphosphonic acid deriv
     prepn
IT   65-85-0, Benzoic acid, reactions   110-90-7D, 1,3,5-Hexahydrotriazine,
     N-polyisobutyl derivs.   532-32-1, Sodium benzoate   589-57-1,
     Diethylchlorophosphite   822-39-9, 2-Chloro-1,3-dioxa-2-
     phospholane   1863-63-4, Ammonium benzoate   3266-66-8
     4560-87-6, 1,3,5-Tris(cyanomethyl)-1,3,5-triazacyclohexane
     5434-82-2 6281-19-2   6286-29-9   7719-12-2,
     Phosphorus chloride (PCl3) 7779-27-3   16887-79-9
     26028-43-3 32468-85-2 58036-76-3   178412-86-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (method for producing α- aminophosphonic acids by the
        reaction of hexahydro triazine derivative with in situ or prepared triorgano
        phosphate)
IT   3348-42-3P 54862-45-2P, Tribenzoyl phosphite
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (method for producing α- aminophosphonic acids by the
        reaction of hexahydro triazine derivative with in situ or prepared triorgano
        phosphate)
IT   98-94-2
     RL: RGT (Reagent); RACT (Reactant or reagent)
        (method for producing α- aminophosphonic acids by the
        reaction of hexahydro triazine derivative with in situ or prepared triorgano
        phosphate)
IT   1066-51-9DP, N-polyisobutyl derivs. 1066-51-9P
     1071-83-6P, Phosphonomethylglycine 53986-91-7P
     56710-63-5P 58327-43-8P 67910-53-6P
     123342-39-2P 134559-78-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (method for producing α- aminophosphonic acids by the
        reaction of hexahydro triazine derivative with in situ or prepared triorgano
        phosphate)
IT   78-87-5, 1,2-Dichloropropane   98-95-3, Nitrobenzene, uses   107-06-2,
     1,2-Dichloroethane, uses   108-88-3, Toluene, uses   123-91-1, Dioxane,
     uses
     RL: NUU (Other use, unclassified); USES (Uses)
        (solvent; method for producing α- aminophosphonic acids
        by the reaction of hexahydro triazine derivative with in situ or prepared
        triorgano phosphate)
RE.CNT  6      THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Basf Ag; WO 0147938 A 2001 HCAPLUS
(2) Courtois, G; SYNTHETIC COMMUNICATIONS 1991, V21(2), P201 HCAPLUS
(3) Maier, L; PHOSPHORUS, SULFUR AND SILICON 1990, V47, P361 HCAPLUS
(4) Monsanto Co; DE 2700017 A 1977 HCAPLUS
(5) Soroka, M; SYNTHESIS 1988, 7, P547
(6) Stevens, C; SYNLETT 1998, 2, P180 HCAPLUS
IT   4560-87-6, 1,3,5-Tris(cyanomethyl)-1,3,5-triazacyclohexane
     5434-82-2 6281-19-2 7779-27-3
     26028-43-3 32468-85-2 58036-76-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (method for producing α- aminophosphonic acids by the
        reaction of hexahydro triazine derivative with in situ or prepared triorgano
        phosphate)
RN   4560-87-6  HCAPLUS
CN   1,3,5-Triazine-1,3,5(2H,4H,6H)-triacetonitrile (9CI)   (CA INDEX NAME)
```



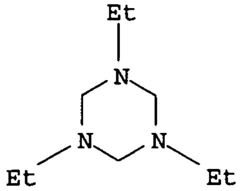
```
RN   5434-82-2  HCAPLUS
CN   1,3,5-Triazine, 1,3,5-tribenzoylhexahydro- (9CI)  (CA INDEX NAME)
```



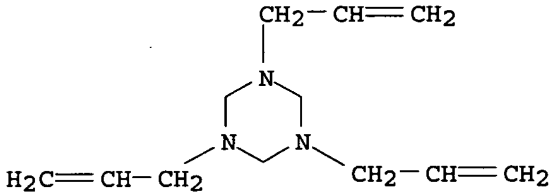
```
RN   6281-19-2  HCAPLUS
CN   1,3,5-Triazine, 1,3,5-tridodecylhexahydro- (9CI)  (CA INDEX NAME)
```



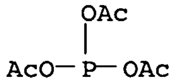
RN 7779-27-3 HCAPLUS
CN 1,3,5-Triazine, 1,3,5-triethylhexahydro- (9CI) (CA INDEX NAME)



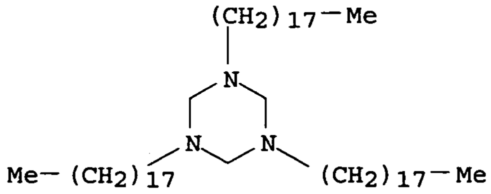
RN 26028-43-3 HCAPLUS
CN 1,3,5-Triazine, hexahydro-1,3,5-tri-2-propenyl- (9CI) (CA INDEX NAME)



RN 32468-85-2 HCAPLUS
CN Acetic acid, trianhydride with phosphorous acid (8CI, 9CI) (CA INDEX NAME)



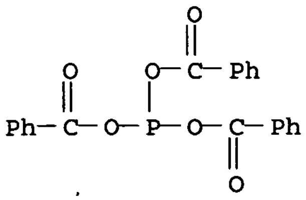
RN 58036-76-3 HCAPLUS
CN 1,3,5-Triazine, hexahydro-1,3,5-trioctadecyl- (9CI) (CA INDEX NAME)



IT **54862-45-2P**, Tribenzoyl **phosphite**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(method for producing α- **aminophosphonic** acids by the

reaction of hexahydro triazine derivative with in situ or prepared triorgano **phosphate**)

RN 54862-45-2 HCAPLUS
CN Benzoic acid, trianhydride with phosphorous acid (9CI) (CA INDEX NAME)



IT **1066-51-9DP**, N-polyisobutyl derivs. **1066-51-9P**
1071-83-6P, **Phosphonomethylglycine** **53986-91-7P**
56710-63-5P **58327-43-8P** **67910-53-6P**
123342-39-2P **134559-78-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(method for producing α- **aminophosphonic** acids by the reaction of hexahydro triazine derivative with in situ or prepared triorgano **phosphate**)

RN 1066-51-9 HCAPLUS
CN Phosphonic acid, (aminomethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$H_2N-CH_2-PO_3H_2$

RN 1066-51-9 HCAPLUS
CN Phosphonic acid, (aminomethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$H_2N-CH_2-PO_3H_2$

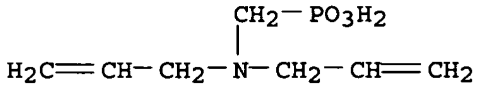
RN 1071-83-6 HCAPLUS
CN Glycine, N-(phosphonomethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

$HO_2C-CH_2-NH-CH_2-PO_3H_2$

RN 53986-91-7 HCAPLUS
CN Phosphonic acid, [(2-propenylamino)methyl]- (9CI) (CA INDEX NAME)

$H_2C=CH-CH_2-NH-CH_2-PO_3H_2$

RN 56710-63-5 HCAPLUS
CN Phosphonic acid, [(di-2-propenylamino)methyl]- (9CI) (CA INDEX NAME)



$H_2C=CH-CH_2-N(CH_2-PO_3H_2)-CH_2-CH=CH_2$

RN 58327-43-8 HCAPLUS
CN Phosphonic acid, [(dodecylamino)methyl]- (9CI) (CA INDEX NAME)

$Me-(CH_2)_{11}-NH-CH_2-PO_3H_2$

```
RN   67910-53-6  HCAPLUS
CN   Phosphonic acid, [(ethylamino)methyl]- (9CI)  (CA INDEX NAME)
```

$EtNH-CH_2-PO_3H_2$

```
RN   123342-39-2  HCAPLUS
CN   Phosphonic acid, [(octadecylamino)methyl]- (9CI)  (CA INDEX NAME)
```

$Me-(CH_2)_{17}-NH-CH_2-PO_3H_2$

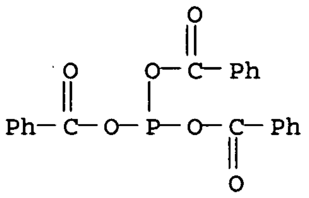
```
RN   134559-78-7  HCAPLUS
CN   Phosphonic acid, [(hydroxyamino)methyl]- (9CI)  (CA INDEX NAME)
```

$HO-NH-CH_2-PO_3H_2$

```
L55  ANSWER 5 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2001:489409  HCAPLUS
DN   135:76990
ED   Entered STN:  06 Jul 2001
TI   Method for production of N-phosphonomethylglycine
IN   Wulff, Christian; Orsten, Stefan; Oftring,
     Alfred
PA   Basf A.-G., Germany
SO   PCT Int. Appl., 31 pp.
     CODEN: PIXXD2
DT   Patent
LA   German
IC   ICM  C07F009-38
     ICS  C07F009-40
CC   29-7 (Organometallic and Organometalloidal Compounds)
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    -------------------    --------
PI   WO 2001047938        A1    20010705    WO 2000-EP13162        20001222 <--
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2395420           AA    20010705    CA 2000-2395420        20001222 <--
     AU 2001057873        A5    20010709    AU 2001-57873          20001222 <--
     AU 779799            B2    20050210
     EP 1240173           A1    20020918    EP 2000-993613         20001222 <--
     EP 1240173           B1    20030514
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2000016668        A     20021008    BR 2000-16668          20001222 <--
     AT 240337            E     20030515    AT 2000-993613         20001222 <--
```

```
          NZ 519593            A      20030530    NZ 2000-519593          20001222 <--
          JP 2003519155        T2     20030617    JP 2001-549408          20001222 <--
          PT 1240173           T      20031031    PT 2000-993613          20001222 <--
          ES 2199898           T3     20040301    ES 2000-993613          20001222 <--
          US 2003004370        A1     20030102    US 2002-168717          20020624 <--
          US 6818793           B2     20041116
          US 2003166966        A1     20030904    US 2003-368577          20030220 <--
          US 6660878           B2     20031209
          US 2004063996        A1     20040401    US 2003-664892          20030922 <--
          US 6855841           B2     20050215
          US 2004092765        A1     20040513    US 2003-678626          20031006 <--
     PRAI DE 1999-19962601     A      19991223  <--
          WO 2000-EP13162      W      20001222  <--
          US 2002-168717       A3     20020624  <--
          US 2003-368577       A3     20030220
     CLASS
      PATENT NO.      CLASS  PATENT FAMILY CLASSIFICATION CODES
      -------------   -----  ----------------------------------------
      WO 2001047938   ICM    C07F009-38
                      ICS    C07F009-40
      WO 2001047938   ECLA   C07F009/38A1+U6F; C07F009/40C9Q                  <--
      US 2003004370   NCL    562/018.000
                      ECLA   C07F009/38A1+U6F; C07F009/40C9Q                  <--
      US 2003166966   NCL    558/386.000; 560/174.000; 562/400.000; 564/123.000;
                             568/008.000
                      ECLA   C07F009/38A1+U6F; C07F009/40C9Q                  <--
      US 2004063996   NCL    562/018.000
                      ECLA   C07F009/38A1+U6F; C07F009/40C9Q                  <--
      US 2004092765   NCL    562/018.000
                      ECLA   C07F009/38A1+U6F; C07F009/40C9Q                  <--
     OS   CASREACT 135:76990
     AB   The invention relates to a method for production of N-
          phosphonomethylglycine, by reaction of a hexahydrotriazine derivative
          with a triacyl phosphite.  The method produces N-
          phosphonomethylglycine in a simple and cost-effective manner and
          in high yield.  Thus, reaction of sodium benzoate with PCl3 in 1,4-dioxane
          followed by treatment with hexahydrotriazine gave 91% N-
          phosphonomethylglycine in 95.3% purity.
     ST   phosphonomethyl glycine prepn; triacyl
          phosphite reaction hexahydrotriazine; triazine hexahydro reaction
          acyl phosphite
     IT   54862-45-2, Tribenzoyl phosphite
          RL: RCT (Reactant); RACT (Reactant or reagent)
             (formation and sequential reaction with hexahydrotriazine in preparation of
             phosphonomethylglycine)
     IT   1071-83-6P, N-Phosphonomethylglycine
          RL: SPN (Synthetic preparation); PREP (Preparation)
             (preparation of)
     IT   98-94-2
          RL: RCT (Reactant); RACT (Reactant or reagent)
             (reaction of phosphorus trichloride with benzoic acid in
             presence of)
     IT   32468-85-2, Tris(acetyloxy)phosphine
          RL: RCT (Reactant); RACT (Reactant or reagent)
             (reaction with hexahydrotriazine in preparation of
             phosphonomethylglycine)
     IT   65-85-0, Benzoic acid, reactions   1863-63-4, Ammonium benzoate
          RL: RCT (Reactant); RACT (Reactant or reagent)
             (reaction with phosphorus trichloride in preparation of
             phosphonomethylglycine)
     IT   7719-12-2, Phosphorus trichloride
          RL: RCT (Reactant); RACT (Reactant or reagent)
             (reaction with sodium benzoate in preparation of
```

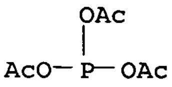
phosphonomethylglycine)
IT **4560-87-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with triacyl **phosphite** in preparation of
phosphonomethylglycine)
IT 532-32-1, Sodium benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequential reaction with **phosphorus** trichloride and
hexahydrotriazine)
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Hyun-Joon, H; US 5053529 A 1991 HCAPLUS
(2) Stauffer Chemical Co; EP 0097522 A 1984 HCAPLUS
(3) Stauffer Chemical Co; EP 0104775 A 1984 HCAPLUS
(4) Stauffer Chemical Co; EP 0149294 A 1985 HCAPLUS
IT **54862-45-2**, Tribenzoyl **phosphite**
RL: RCT (Reactant); RACT (Reactant or reagent)
(formation and sequential reaction with hexahydrotriazine in preparation of
phosphonomethylglycine)
RN 54862-45-2 HCAPLUS
CN Benzoic acid, trianhydride with phosphorous acid (9CI) (CA INDEX NAME)



IT **1071-83-6P**, N-**Phosphonomethylglycine**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 1071-83-6 HCAPLUS
CN Glycine, N-(phosphonomethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

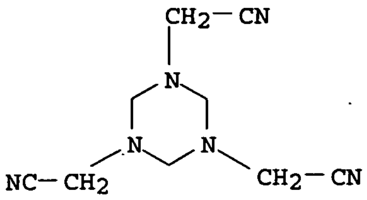
$HO_2C—CH_2—NH—CH_2—PO_3H_2$

IT **32468-85-2**, Tris(acetyloxy)**phosphine**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with hexahydrotriazine in preparation of
phosphonomethylglycine)
RN 32468-85-2 HCAPLUS
CN Acetic acid, trianhydride with phosphorous acid (8CI, 9CI) (CA INDEX
NAME)

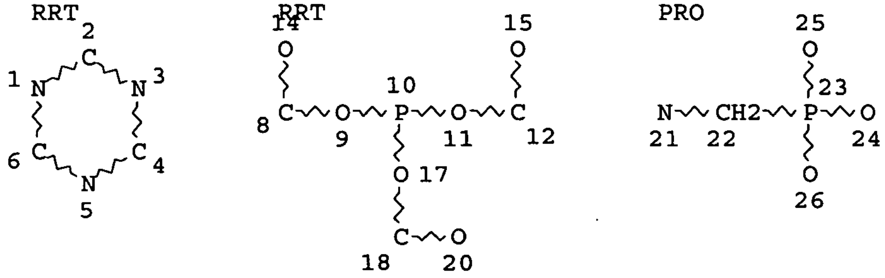


$P(OAc)_3$

IT **4560-87-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with triacyl **phosphite** in preparation of
phosphonomethylglycine)
RN 4560-87-6 HCAPLUS
CN 1,3,5-Triazine-1,3,5(2H,4H,6H)-triacetonitrile (9CI) (CA INDEX NAME)

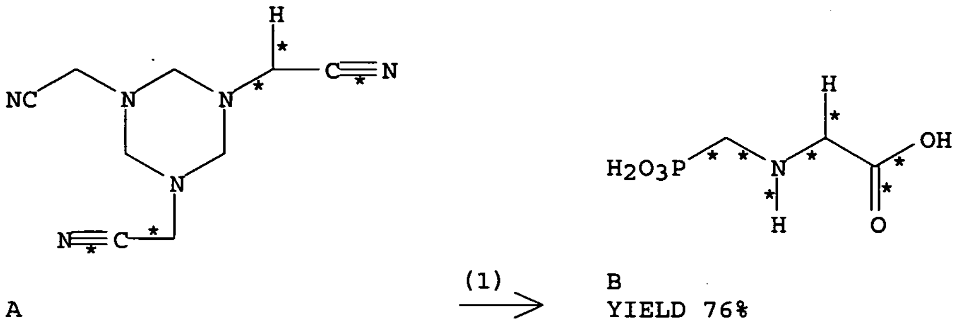


```
=> => fil casreact
FILE 'CASREACT' ENTERED AT 09:05:33 ON 03 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 1 May 2005 VOL 142 ISS 18

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 9.2 million reactions      *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d sta que
L58                STR
```



```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1
NUMBER OF NODES IS  22

STEREO ATTRIBUTES: NONE
L60             2 SEA FILE=CASREACT SSS FUL L58 (      2 REACTIONS)
```

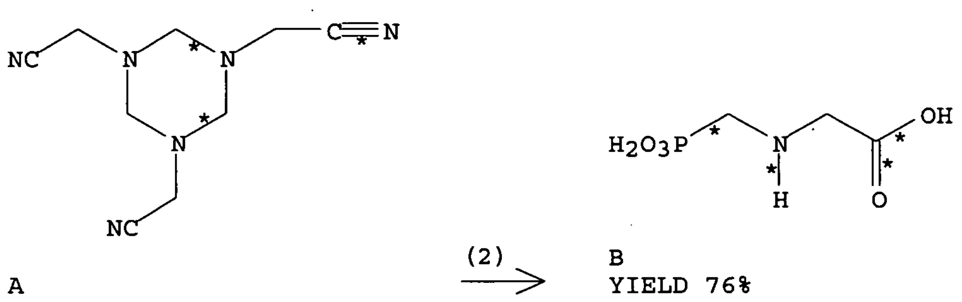
```
100.0% DONE      19 VERIFIED        2 HIT RXNS                         2 DOCS
SEARCH TIME: 00.00.01


=> d bib abs fhit retable tot


L60  ANSWER 1 OF 2  CASREACT  COPYRIGHT 2005 ACS on STN
AN   138:56079  CASREACT
TI   Method for producing α-aminophosphonic acids by the reaction of
     hexahydro triazine derivative with triorgano phosphate
IN   Wulff, Christian; Orsten, Stefan; Oftring, Alfred
PA   BASF Aktiengesellschaft, Germany
SO   PCT Int. Appl., 43 pp.
     CODEN: PIXXD2
DT   Patent
LA   German
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
PI   WO 2003000702      A1   20030103       WO 2002-EP6901   20020621
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10130134        A1   20030102       DE 2001-10130134 20010622
     EP 1401847         A1   20040331       EP 2002-780837   20020621
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2002010528      A    20040622       BR 2002-10528    20020621
     US 2004236144      A1   20041125       US 2003-481576   20031222
PRAI DE 2001-10130134  20010622
     WO 2002-EP6901   20020621
OS   MARPAT 138:56079
AB   The invention relates to a method for producing α-aminophosphonic
     acids, by reacting a hexahydro triazine derivative with a triorgano phosphate.
     The inventive method includes a phosphono compound as an intermediate step,
     said phosphono compound being hydrolyzed into α-aminophosphonic acid.
     The invention also relates to said phosphono compound and the method for the
     production thereof.  Thus, reaction of PCl3 with sodium benzoate in
     1,4-dioxane followed by treatment with 1,3,5-tris(cyanomethyl)-1,3,5-
     triazacyclohexane and aqueous HCl hydrolysis gave 91% phosphonomethylglycine
     in 95.3% purity.  The inventive method enables α-aminophosphonic
     acids to be produced in a simple and economical manner as well as ensuring
     a high yield and purity.


RX(1) OF 16     A  ===>  B
```



A

B
YIELD 76%

```
RX(1)      RCT  A 4560-87-6

             STAGE(1)
                RGT  C 32468-85-2 Acetic acid, trianhydride with
                          phosphorous acid
                SOL  123-91-1 Dioxane

             STAGE(2)
                RGT  D 7647-01-0 HCl
                SOL  7732-18-5 Water
           PRO  B 1071-83-6
RETABLE
   Referenced Author    |Year | VOL | PG  | Referenced Work    | Referenced
         (RAU)          |(RPY)|(RVL)|(RPG)|       (RWK)        | File
========================+=====+=====+=====+====================+==========
Basf Ag                 |2001 |     |     |WO 0147938 A        |CAPLUS
Courtois, G             |1991 |21   |201  |SYNTHETIC COMMUNICAT|CAPLUS
Maier, L                |1990 |47   |361  |PHOSPHORUS, SULFUR A|CAPLUS
Monsanto Co             |1977 |     |     |DE 2700017 A        |CAPLUS
Soroka, M               |1988 |     |547  |SYNTHESIS           |
Stevens, C              |1998 |     |180  |SYNLETT             |CAPLUS


L60  ANSWER 2 OF 2  CASREACT  COPYRIGHT 2005 ACS on STN
AN   135:76990  CASREACT
TI   Method for production of N-phosphonomethylglycine
IN   Wulff, Christian; Orsten, Stefan; Oftring, Alfred
PA   Basf A.-G., Germany
SO   PCT Int. Appl., 31 pp.
     CODEN: PIXXD2
DT   Patent
LA   German
FAN.CNT 1
     PATENT NO.          KIND  DATE          APPLICATION NO.  DATE
     ---------------     ----  --------      ---------------  --------
PI   WO 2001047938        A1   20010705      WO 2000-EP13162  20001222
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2395420           AA   20010705      CA 2000-2395420  20001222
     AU 2001057873        A5   20010709      AU 2001-57873    20001222
     AU 779799           B2    20050210
     EP 1240173          A1    20020918          EP 2000-993613    20001222
     EP 1240173          B1    20030514
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     BR 2000016668       A     20021008          BR 2000-16668     20001222
     AT 240337           E     20030515          AT 2000-993613    20001222
     NZ 519593           A     20030530          NZ 2000-519593    20001222
     JP 2003519155       T2    20030617          JP 2001-549408    20001222
     PT 1240173          T     20031031          PT 2000-993613    20001222
     ES 2199898          T3    20040301          ES 2000-993613    20001222
     US 2003004370       A1    20030102          US 2002-168717    20020624
     US 6818793          B2    20041116
     US 2003166966       A1    20030904          US 2003-368577    20030220
     US 6660878          B2    20031209
     US 2004063996       A1    20040401          US 2003-664892    20030922
     US 6855841          B2    20050215
     US 2004092765       A1    20040513          US 2003-678626    20031006
PRAI DE 1999-19962601  19991223
     WO 2000-EP13162   20001222
     US 2002-168717    20020624
     US 2003-368577    20030220
AB   The invention relates to a method for production of N-phosphonomethylglycine,
     by reaction of a hexahydrotriazine derivative with a triacyl phosphite.  The
     method produces N-phosphonomethylglycine in a simple and cost-effective
     manner and in high yield.  Thus, reaction of sodium benzoate with PCl3 in
     1,4-dioxane followed by treatment with hexahydrotriazine gave 91%
     N-phosphonomethylglycine in 95.3% purity.


RX(2) OF 2      A  ===>  B
```



```
RX(2)       RCT  A 4560-87-6
            RGT  F 32468-85-2 Acetic acid, trianhydride with
                 phosphorous acid
            PRO  B 1071-83-6
            SOL  123-91-1 Dioxane
RETABLE
   Referenced Author    |Year | VOL | PG  | Referenced Work    | Referenced
        (RAU)           |(RPY)|(RVL)|(RPG)|      (RWK)         | File
=====================+=====+=====+======+====================+==========
Hyun-Joon, H          |1991 |     |      |US 5053529 A        |CAPLUS
Stauffer Chemical Co  |1984 |     |      |EP 0097522 A        |CAPLUS
Stauffer Chemical Co  |1984 |     |      |EP 0104775 A        |CAPLUS
Stauffer Chemical Co  |1985 |     |      |EP 0149294 A        |CAPLUS


=> d his

     (FILE 'HOME' ENTERED AT 08:39:10 ON 03 MAY 2005)
```

```
                SET COST OFF

     FILE 'HCAPLUS' ENTERED AT 08:40:08 ON 03 MAY 2005
L1            1 S US20040092765/PN OR (US2003-678626# OR WO2000-EP13162 OR US20
                E WULFF C/AU
L2           56 S E3,E4,E9,E10
                E ORSTEN S/AU
L3            8 S E4
                E OFTRING A/AU
L4          130 S E3,E4
                E OEFTRING A/AU
                E OFFTRING/AU
L5            4 S L2-L4 AND ?PHOSPHONOMETHYLGLYCIN?
L6           16 S L2-L4 AND ?GLYCIN?
L7            5 S L6 AND ?PHOSPH?
L8            5 S L5,L7
L9            4 S L2-L4 AND ?PHOSPHONOMETHYL GLYCIN?
L10           0 S L2-L4 AND ?PHOSPHONO METHYL GLYCIN?
L11           0 S L2-L4 AND ?PHOSPHONO METHYLGLYCIN?
L12           5 S L8,L9
                SEL RN

     FILE 'REGISTRY' ENTERED AT 08:47:11 ON 03 MAY 2005
L13         118 S E1-E118
L14           1 S 1071-83-6
L15         739 S 1071-83-6/CRN

     FILE 'HCAPLUS' ENTERED AT 08:47:33 ON 03 MAY 2005
L16        5180 S L14
L17        1411 S L15
L18           5 S L2-L4 AND L16,L17
L19           5 S L12,L18

     FILE 'REGISTRY' ENTERED AT 08:47:53 ON 03 MAY 2005
L20           1 S L13 AND L14,L15
L21         117 S L13 NOT L20
L22           8 S L21 AND NCNCNC/ES
L23          15 S L21 AND P/ELS
L24           3 S L23 AND O>=6
L25           2 S L24 NOT N/ELS
L26             STR
L27          50 S L26
L28       11337 S L26 FUL
L29           1 S L22 AND C9H12N6
L30       11337 S L28,L29
L31           2 S L22 NOT L30
L32             STR
L33           3 S L32
L34          44 S L32 FUL
                SAV L28 SHIAO678A/A
                SAV L34 SHIAO678B/A
L35             STR
L36             STR L35
L37          50 S L36
L38        8960 S L36 FUL
                SAV L38 SHIAO678C/A
L39           0 S L35 FUL SUB=L38
L40           9 S L13 AND L38
L41           2 S L13 AND L34

     FILE 'HCAPLUS' ENTERED AT 08:57:41 ON 03 MAY 2005
L42       14182 S L30
L43          50 S L34
```

```
L44            2 S L42 AND L43
L45            2 S L44 AND L16,L17
L46            2 S L44 AND L38
L47            2 S L44 AND (?PHOSPHONOMETHYLGLYCIN? OR ?PHOSPHONOMETHYL GLYCIN?
L48            2 S L44-L47
L49            2 S L48 AND L1-L12
L50            2 S L19 AND L49
L51            3 S L19 NOT L50
L52            4 S L1-L12 AND L42
L53            2 S L1-L12 AND L43
L54            5 S L1-L12 AND L38
L55            5 S L12,L19,L50-L54

     FILE 'REGISTRY' ENTERED AT 09:00:59 ON 03 MAY 2005

     FILE 'HCAPLUS' ENTERED AT 09:01:32 ON 03 MAY 2005

     FILE 'CASREACT' ENTERED AT 09:02:07 ON 03 MAY 2005
L56              STR
L57            0 S L56
L58              STR L56
L59            0 S L58
L60            2 S L58 FUL
                 SAV L60 SHIAO678D/A

     FILE 'CASREACT' ENTERED AT 09:05:33 ON 03 MAY 2005

=>
```